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Diffuse interface approach to CFD-based simulation of gas-liquid systems

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Diffuse Interface Approach to CFD-Based Simulation of Gas-Liquid Systems

A. Donaldson, A. Macchi, D.M. Kirpalani*
CSCHE 2008, Ottawa, ON
October 21, 2008

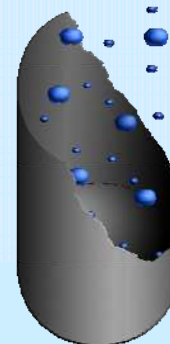
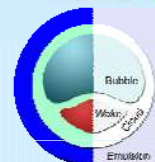


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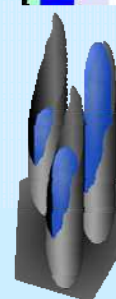
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Miniaturization and Multi-phase CFD



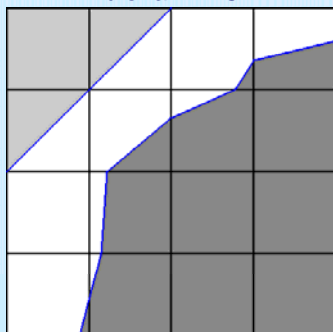
- Process intensification and miniaturization has led to alternative technologies for multi-phase contacting (i.e. monoliths)
- The modular nature of this technology is better suited to CFD-based optimization, where the process dynamics remain consistent during industrial scale-up.
- Simulation of interfacial phenomena in small-scale geometries is complicated by a change in the predominant forces acting on the fluids.



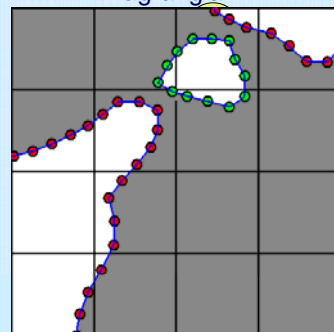
Multi-Phase CFD: Sharp Interface

Sharp interface tracking methods describe the transition between phases as a discontinuity, from which topology is reconstructed to evaluate property transitions and surface forces.

Eulerian - VOF

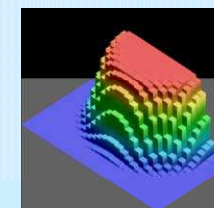
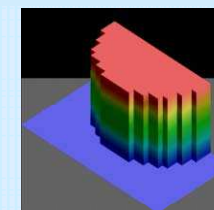


Lagrangian



Diffuse Interface Approach

- The interface between phases is described as a region of finite width, across which physical properties transition smoothly
- Phase interactions are described by resolving thermodynamic relationships within the artificially thickened interface.
- Surface forces are evaluated as a function of free energy variation, eliminating the need to reconstruct the interface geometry.
- Topological changes are handled implicitly

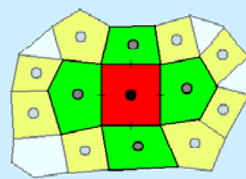
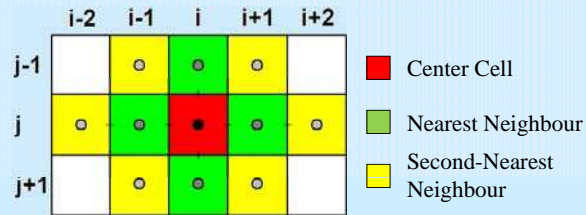


DI Approach: Current Limitations

Spontaneous Drop Shrinkage and Continuity Loss:

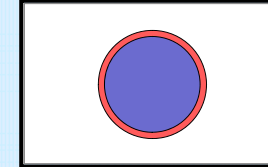
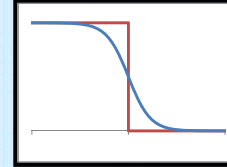
When the DI approach is used as an interface tracking technique, the contour $\phi = 0.5$ is frequently used to delineate between phases. While ϕ is conserved, the area within the contour is not.

Application To Non-Uniform Meshes and Surface Force Approximations

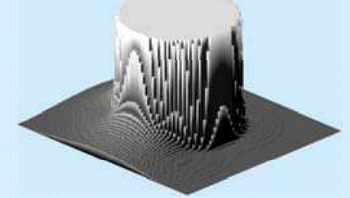


Continuity Loss: Sources and Effects

Initial Conditioning:



Loss During Advection:

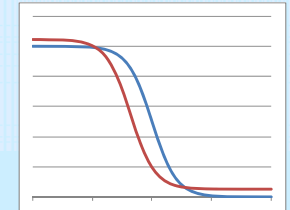


Spontaneous Drop Shrinkage:

$$H(\phi) = \int_V \text{Surface Energy} + \text{Bulk Free Energy}$$

Assume: Negligible Volume, Near Zero Infinite Volume, Dominant energy

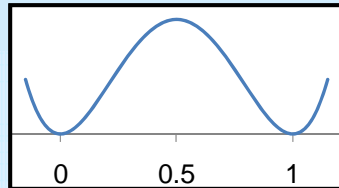
Reality: Concentration of Free Energy on Interface Finite Volume, Near Zero



Conventional Approach: Double-Well Function

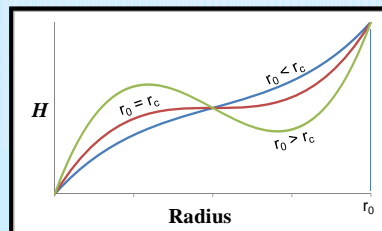
Simplified Energy Density Function:

$$f_{\text{Double-Well}}(\phi) = 0.25\phi^2(1-\phi)^2$$



Spontaneous Drop Shrinkage: Critical Radius 2-D

For a set interface width and computational domain volume, a critical droplet radius exists, below which a droplet will eventually disappear.



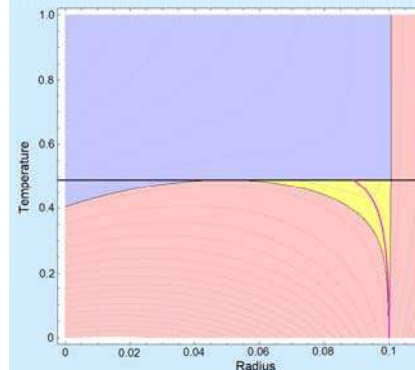
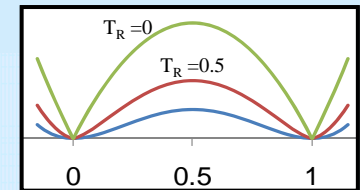
$$r_c \approx \left(\frac{\sqrt{6}}{8\pi} V \varepsilon \right)^{1/3}$$

Yue et al., J. Comp. Phys., 223 (2007)

Proposed Approach: TVSED Function

Temperature Variant SEDFunction:

$$f_{\text{TVSED}}(\phi) = |\phi(1-\phi)|^{1+T_R}$$



Critical Radius – 2D

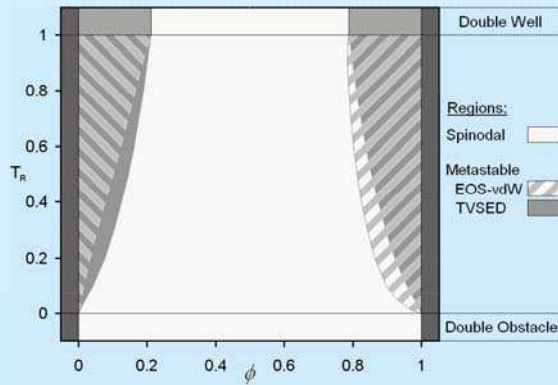
$$r_c = \left[\frac{\sqrt{1+2T_R}}{\sqrt{2(T_R+1)}} \left(\frac{1+2T_R}{4T_R} \frac{V}{\pi} \right)^{T_R} \dots \right]^{\frac{1}{2T_R+1}}$$

$$\dots \varepsilon {}_2F_1 \left[\frac{1}{2}, -\frac{(1+T_R)}{2}; \frac{3}{2}; 1 \right]$$

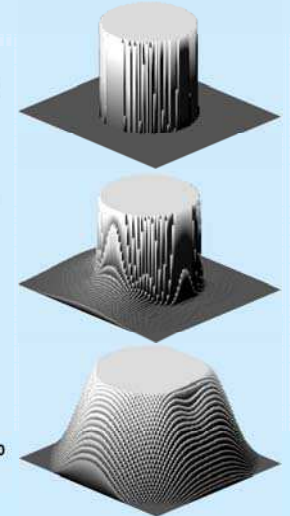
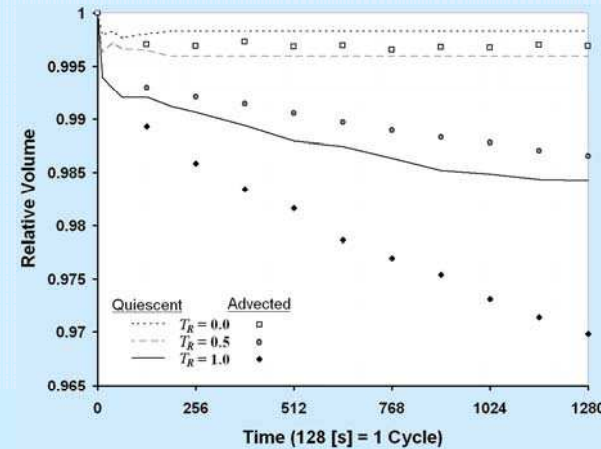
Continuity Loss During Advection

Continuity loss during advection occurs due to the formation of meta-stable mixtures in the bulk phases, caused by poor separation dynamics.

Thermodynamic Regions



Diagonal Advection Simulations



Two-Phase Flow: Momentum Transfer

Navier-Stokes for Laminar Flow:

$$\rho \left[\frac{\partial U}{\partial t} + \nabla \cdot (UU) \right] = -\nabla \cdot P + \nabla \cdot [\mu (\nabla U + \nabla U^T)] - \rho \bar{g}$$

Continuity:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$

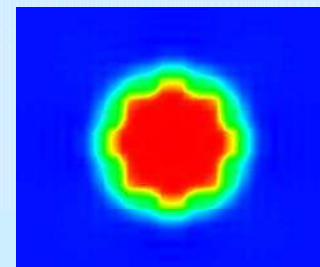
Surface forces accounted for in the pressure tensor.

Note: As per Ding et al. (2007), the volume averaged velocity is used to obtain a solenoidal velocity field, thereby simplifying the PISO algorithm used for determining the pressure field.

Pressure Tensor: Surface Force Est.

The pressure tensor for diffuse interface simulations is commonly based on the Korteweg tensor, with isotropic terms incorporated into the isotropic pressure, p .

$$\nabla \cdot P = \nabla p - \lambda (\nabla (\nabla \phi)^2) - \nabla \cdot (\nabla \phi \otimes \nabla \phi)$$

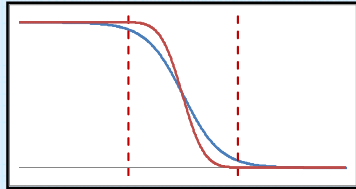


Surface Force and Gamma Filtering

By applying a filter to ϕ , variations in the pressure tensor can be localized to the center of the interface where ϕ is more linear, minimizing the error introduced by low-order estimates of $\nabla\phi$

$$\phi^* = 0.5 + 0.5 \sin(\theta)$$

$$\theta = [\min(\max(\phi, \varphi), 1 - \varphi) - 0.5] \frac{\pi}{1 - 2\varphi}$$



$$\nabla \cdot P = \nabla p - \lambda^* \left[\nabla \left(|\nabla \phi^*|^2 \right) - \nabla \cdot (\nabla \phi^* \otimes \nabla \phi^*) \right]$$

$$\lambda^* \nabla \left(|\nabla \phi^*|^2 \right) = \lambda^* 2\beta |\cos(\theta) \nabla \phi| \left\{ \cos(\theta) \nabla |\nabla \phi| - \delta_\phi 2\sqrt{\beta} |\nabla \phi| \sin(\theta) \nabla \phi \right\}$$

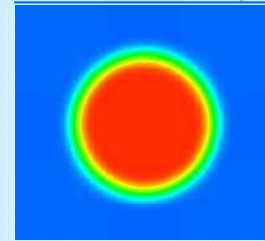
$$\beta = \left(\frac{\pi}{2(1-2\varphi)} \right)^2$$

$$\delta_\phi = \begin{cases} 1 & \varphi < \phi < 1-\varphi \\ 0 & \phi \geq 1-\varphi, \phi \leq \varphi \end{cases}$$

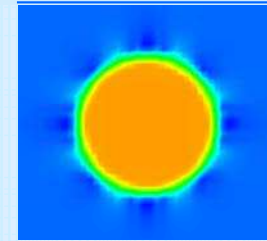
$$\lambda^* \nabla \cdot (\nabla \phi^* \otimes \nabla \phi^*) = \lambda^* \beta \left\{ \cos^2(\theta) \left[(\nabla^2 \phi) (\nabla \phi) + (\nabla \phi) \cdot \nabla (\nabla \phi) \right] - 2\sqrt{\beta} \sin(2\theta) (\nabla \phi \otimes \nabla \phi) \cdot \nabla \phi \right\}$$

Surface Force Results

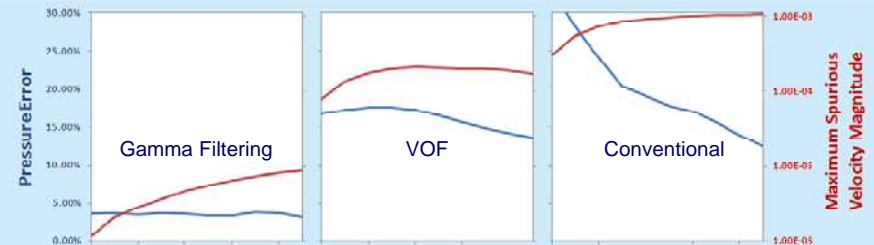
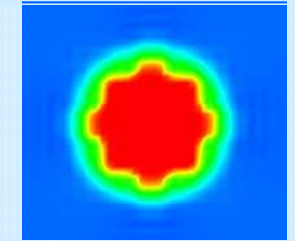
Gamma Filtering



VOF



Conventional



Summary

- While the diffuse interface approach to interface tracking has advantages over the sharp interface approach for modeling small-scale flows, its application has been limited due to continuity losses and the need for highly structured grids.
- The current practice of adopting the double-well function is partially responsible for the observed loss in continuity. By using an energy density for immiscible fluids, overall phase continuity is improved.
- Estimates for pressure can be improved through the use of a filtering parameter, limiting pressure variations to the central region of the interface where the equilibrium profile is linear.
- These improvements enable the use of the diffuse interface technique on unstructured grids, a requirement for most practical applications where it may be of use.

Questions?

Scalar Transport Equations:

Convective Cahn-Hilliard Equation:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi U) + \nabla \cdot (\Gamma J) = 0$$

Diffusive Flux, J , maintains the interface profile through chemical potential gradients, $\nabla \eta$:

$$J = -\nabla \eta = \frac{\lambda}{\varepsilon^2} (\varepsilon^2 \nabla (\nabla^2 \phi) - f''(\phi) \nabla \phi)$$

ε - Capillary Width

λ - Mixing Energy Density

f - Free energy density governing interfacial dynamics and the equilibrium profile of

Multi-Phase CFD: Approach Limitations

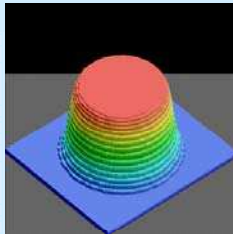
The ability of each method to resolve complex multi-phase flow is often limited by shortcomings inherent to the numerical approach.

Lagrangian	Eulerian	
	Front Tracking	Sharp Interface (VOF) / Diffuse Interface (PF)
<ul style="list-style-type: none"> • Book keeping • Complex Topology • Coalescence & Breakup • CSF model 	<ul style="list-style-type: none"> • CSF model • Coal. & Breakup • Interface smearing and reconstruction 	<ul style="list-style-type: none"> • Larger grid needed to resolve interface • 4th order derivative → High order schemes • Spontaneous drop shrinkage

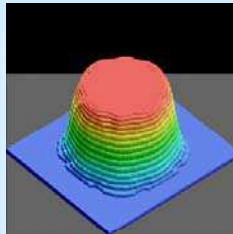
While a number of these limitations have been addressed, the associated increase in complexity often results in a method which is too cumbersome for general application to multi-phase flow problems.

Pressure Profiles: Method Comparison

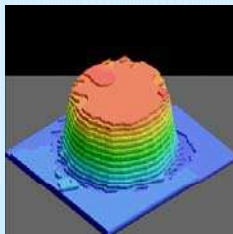
Phase Field



Grad Gamma



VOF



CSF-Kim

